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Lindemann-Gilvarry melting law and Debye temperatures of cubic semiconductors

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Lindemann's theory (1910) of fusion for monatomic solids assumes that melting occurs when the amplitude of thermal vibrations of the atoms reach one half the distance of separation of neighbouring atoms less their diameter. Gilvarry (1956), however, suggested that fusion occurs when the ratio of the root-mean square amplitude of thermal vibration $< u_{av}^2 >$ to the square of the nearest neighbour separation δ, reaches a certain critical fraction; this fraction is presumed to be the same for all solids To estimate the amplitude of thermal vibration, one can make use of the Debye-Waller theory of the temperature factor of X-ray scattering.

$$< u_{av}^2 > = \frac{3h^2T}{4\pi^2mk\Theta^2}\left[x^{-1}\int_0^x y(e^y-1)^{-1}dy + \frac{x}{4}\right] \quad \ldots (1)$$

where $x = \Theta/T$.

For x small, the term within the bracket is approximately unity The Debye temperature Θ, can then be computed from the relation

$$\frac{< u_{av}^2 >}{\delta^2} = \eta = \frac{3h^2T_m}{4\pi^2mk\Theta^2\delta^2}$$

$$= \frac{145.5T_m}{\Theta^2A\delta^2} \quad \ldots (2)$$

where T_m is the melting point, A the atomic weight and δ is expressed in angstroms.

The above relation has been used by Sirota (1968) to calculate the Debye temperatures of $A^{III}B^{V}$ group of semiconductors, taking germanium as the reference element to determine the value of the constant η. The validity of the assumption of constant η has been investigated by Singh & Sharma (1968) for a number of cubic elements and it has been found that η has nearly the same value for elements of a particular group of the Periodic Table but exhibits wide variation from one group to another The same conclusion is also borne out for $A^{III}B^{V}$ and $A^{II}B^{VI}$ groups of semiconductors as shown in table 1. The choice of germanium as the reference element for determining the constant η does not, therefore, seem to be justified. A mean value of η obtained from known compounds is

expected to yield better agreement and should be used for calculating Θ values for that group of compounds.

Table 1. η values for $A^{III}B^{V}$ and $A^{II}B^{VI}$ semiconductors

Compound	T_m (°K)	Θ (°K)	η (10^{-3})	Compound	T_m (°K)	Θ (°K)	η (10^{-3})
AlSb	1327	296 8	4.182	ZnS	1923	347.1	8.702
GaP	1623	445.4	4 250	ZnSe	1788	278.1	7 749
GaAs	1510	344 0	4 281	ZnTe	1568	225 1	6 685
GaSb	985	267.4	3 005	CdSe	1625	230.0	6.730
InP	1327	303 4	4 458	CdTe	1371	163 5	7 902
InAs	1216	251 3	4 298	HgSe	1038	152 3	6 733
InSb	798	201 5	3 071	HgTe	943	142.2	5 337

Relation (2) has been used to obtain a rough estimate of the Debye temperatures of semiconducting compounds AlAs, AlP, and BP for which Θ values are not available in the literature. The Debye temperatures thus estimated are 455, 648 and 977°K, respectively, and these values are in fair agreement to those (417, 588 and 985°K) predicted from lattice constant data (Steigmeier 1963, Aggarwal *et al* 1972) The differences can be attributed to the uncertainty in the values of the melting points of these compounds.

It is, however, to be emphasized that the Lindemann-Gilvarry theory developed for cubic monatomic solids may be applied to compounds only for approximate evaluation. Not only the Debye temperature is a function of temperature but the available experimental data also reveal that the value of $< u_{av}^2 >$ close to the melting point, differs considerably from the theoretical value (*cf.* Viswamitra & Jayalakshmi, 1970). No great accracy should, therfore, be expected from this method but the method is still useful in predicting unknown Debye temperatures.

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